Ensemble Learning

CS4780/5780 – Machine Learning
Fall 2013

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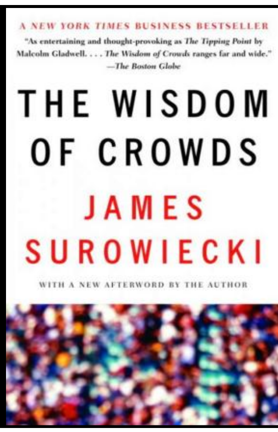
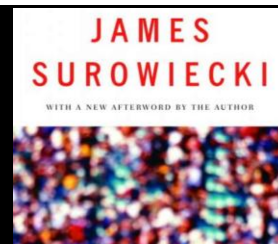
Cornell University

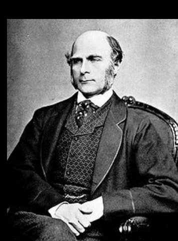
Ensemble Learning

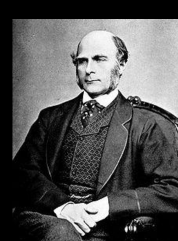
A class of “meta” learning algorithms



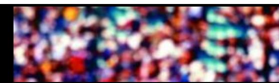


“*The Wisdom of Crowds: Why the Many Are Smarter Than the Few and How Collective Wisdom Shapes Business, Economies, Societies and Nations*”





1,198 lb 1,197 lb



Criteria	Description
Diversity of opinion	*Each person should have private information even if it's just an eccentric interpretation of the known facts.*
Independence	*People's opinions aren't determined by the opinions of those around them.*
Decentralization	*People are able to specialize and draw on local knowledge.*
Aggregation	*Some mechanism exists for turning private judgments into a collective decision.*

Ensemble Learning

A class of "meta" learning algorithms

Combining multiple classifiers to increase performance

Very effective in practice

Good theoretical guarantees

Easy to implement!

Ensemble

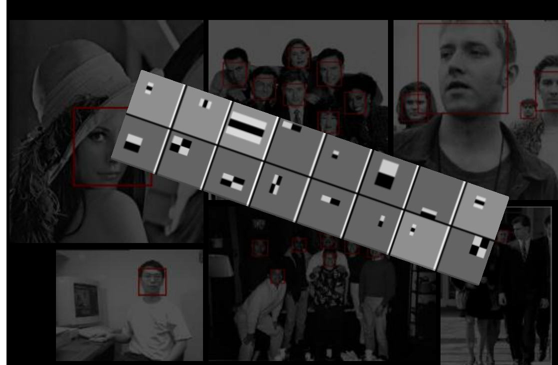
Problem : given *T* binary classification hypotheses (h_1,..., h_T), **find** a combined classifier:

$$h_S(x) = \text{sign}\left(\sum_{t=1}^{T} \alpha_t h_t(x)\right)$$

with better performance.

Teaser

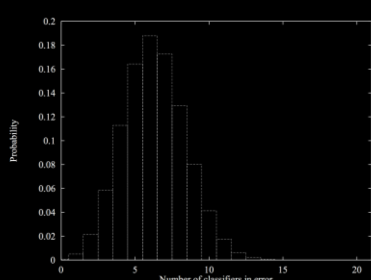
Teaser



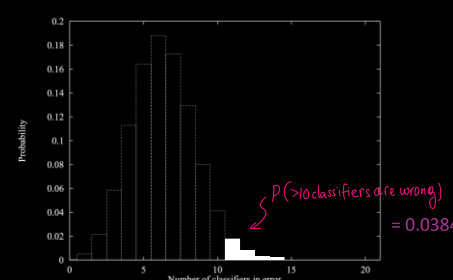
Why do Ensembles work?

Hypothetical Classifier with $P_{error} = 0.3$

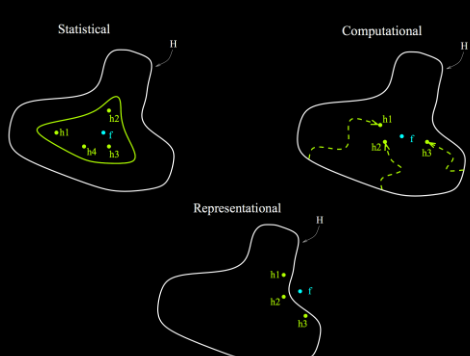
Hypothetical Classifier with $P_{error} = 0.3$



Hypothetical Classifier with $P_{error} = 0.3$



Why do Ensembles work?



BAGGING

Bagging

Bagging (Boostrap aggregating). (Breiman, 1996)

BAGGING$(S=((x_1,y_1),\ldots,(x_m,y_m)))$
for $t \leftarrow 1$ **to** T **do**
  $S_t \leftarrow$ BOOTSTRAP(S) ▷ i.i.d. sampling with replacement from S.
  $h_t \leftarrow$ TRAINCLASSIFIER(S_t)
return $h_S = x \mapsto$ MAJORITYVOTE$((h_1(x),\ldots,h_T(x)))$

Bagging

Ensemble :

$$h_S(x) = \text{sign}\left(\sum_{t=1}^{T} \alpha_t h_t(x)\right)$$

Bagging : Special case where we fix:

$$\alpha_t = 1 \quad \text{and} \quad h_t = \mathbb{L}(S_t)^{*}$$

* $\mathbb{L}$ is some learning algorithm

S_t is a training set drawn from distribution $P(<x,y>)$

Bias-Variance Tradeoff

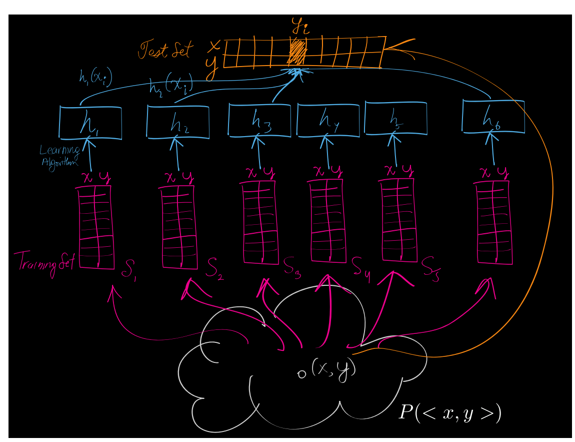
Generalization Error

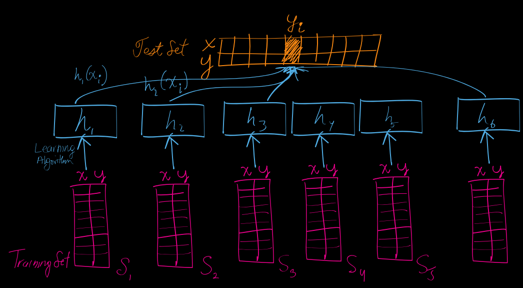
Classification :

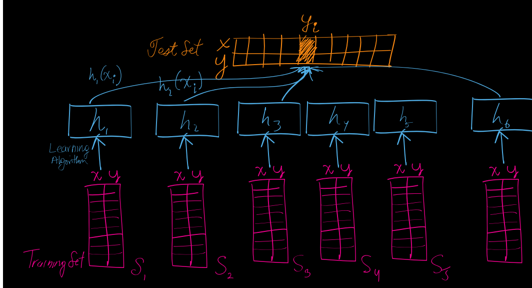
$$\epsilon_{test} = \frac{1}{n}\sum_{i}^{n} \text{Zero-One-Loss}(y_i, h(x_i))$$

Regression :

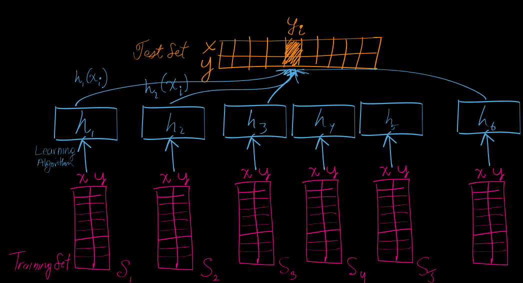
$$\epsilon_{test} = \frac{1}{n}\sum_{i}^{n} (y_i - h(x_i))^2$$







$$\bar{\epsilon}_{test}(x_i) = \frac{1}{T}\sum_{t}^{T}(y_i - h_t(x_i))^2$$



$$\bar{\epsilon}_{test}(x_i) = \frac{1}{T}\sum_{t}^{T}(y_i - h_t(x_i))^2$$

OR, as an expectation:

$$\mathbb{E}_S\left[(y_i - h_S(x_i))^2\right]$$

For the entire test set:

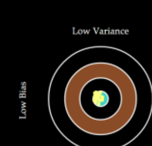
$$\mathbb{E}_{X,Y}\mathbb{E}_S\left[(y_i - h_S(x_i))^2\right]$$

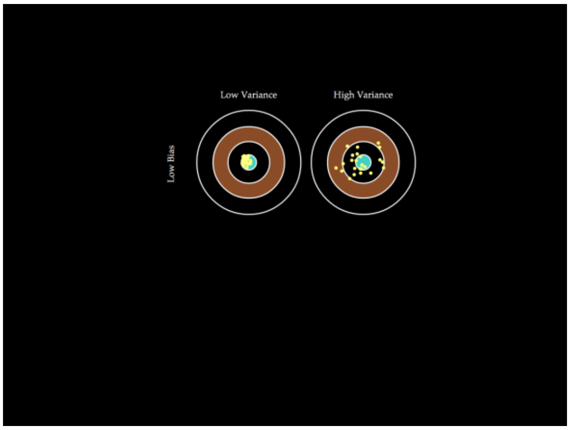
CLAIM:

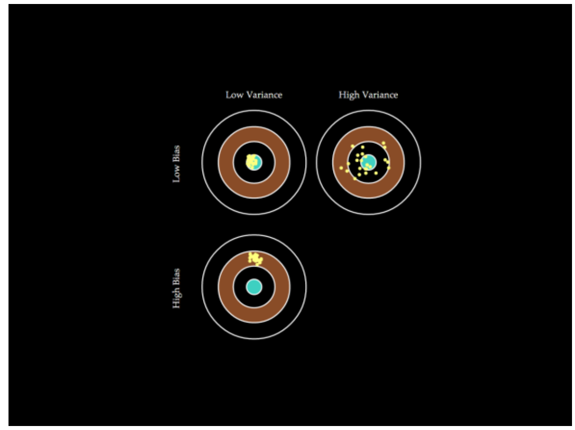
$$\mathbb{E}_S\left[(y_i - h_S(x_i))^2\right] =$$

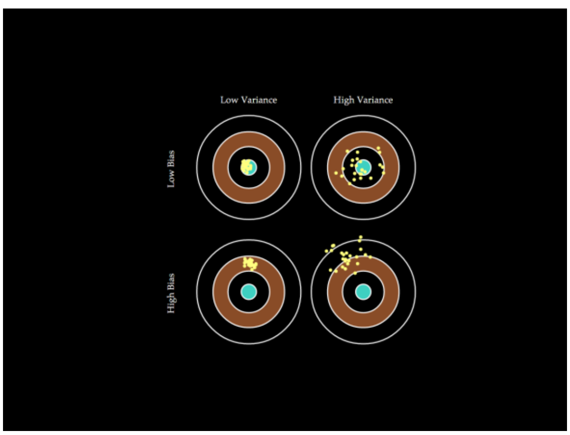
bias² $(y_i - \mathbb{E}_S[h_S(x_i)])^2 \; +$

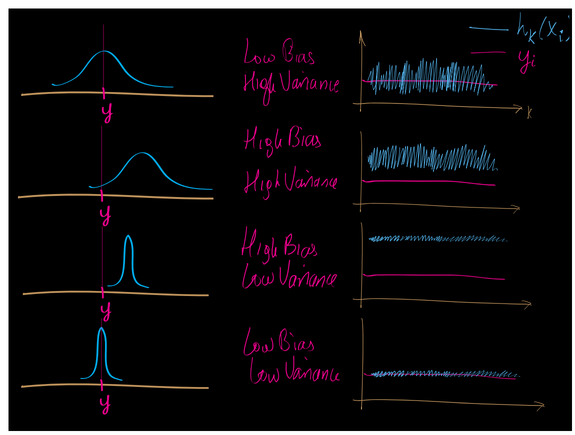
variance $+ \; \mathbb{E}_S[(h_s(x_i) - \mathbb{E}_S[(h_S(x_i))])^2]$

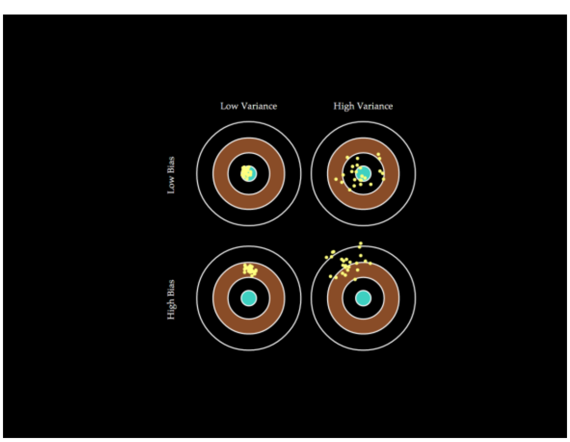


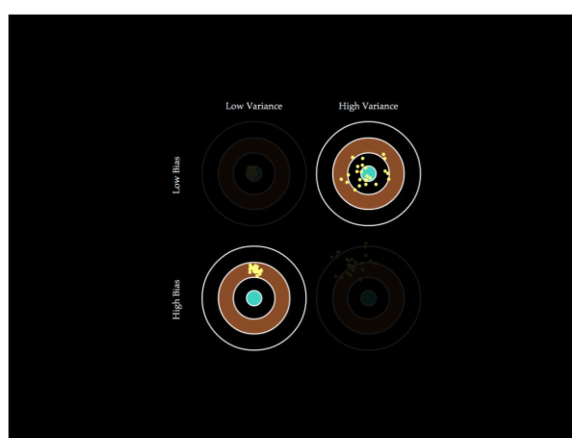

Low Variance
High Variance
Low Bias

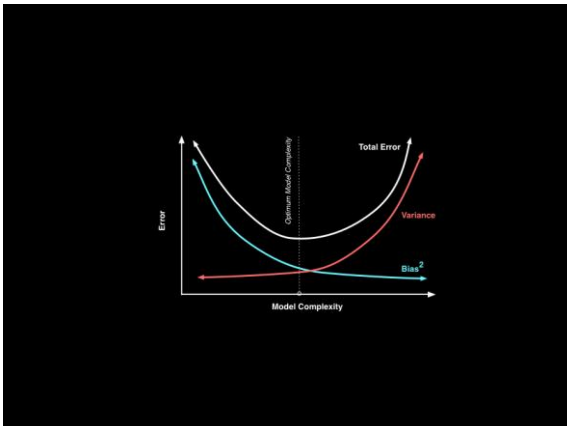

Low Variance
High Variance
Low Bias
High Bias

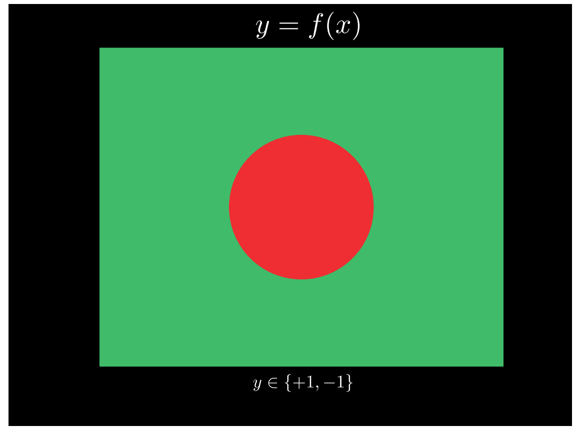

Low Variance
High Variance
Low Bias
High Bias

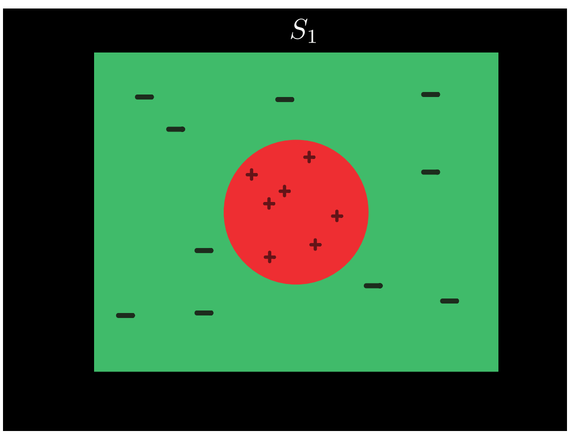

Low Bias
High Variance
High Bias
High Variance
High Bias
Low Variance
Low Bias
Low Variance

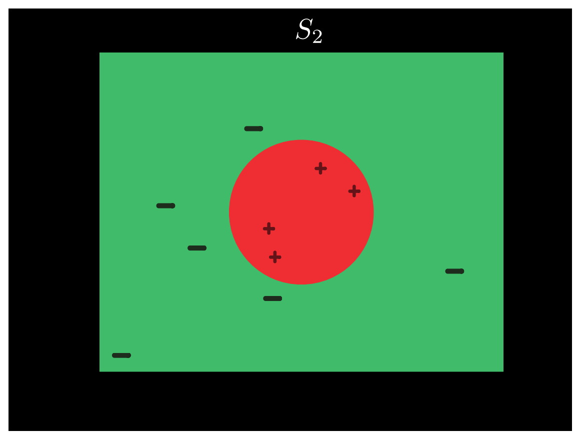

Low Variance
High Variance
Low Bias
High Bias

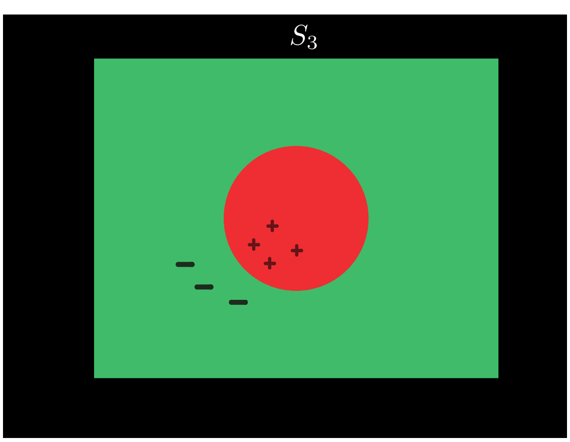

Low Variance
High Variance
Low Bias
High Bias

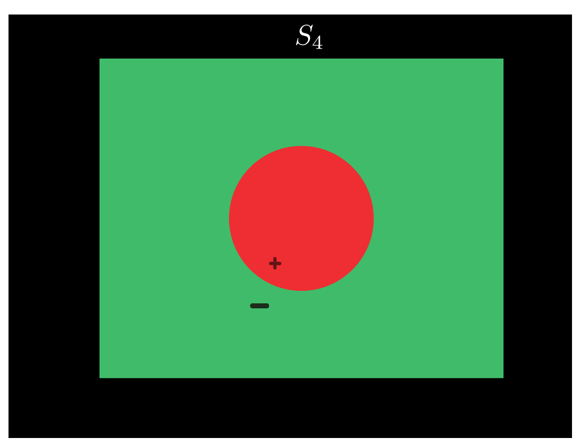

Total Error
Variance
Bias^2
Optimum Model Complexity
Error
Model Complexity

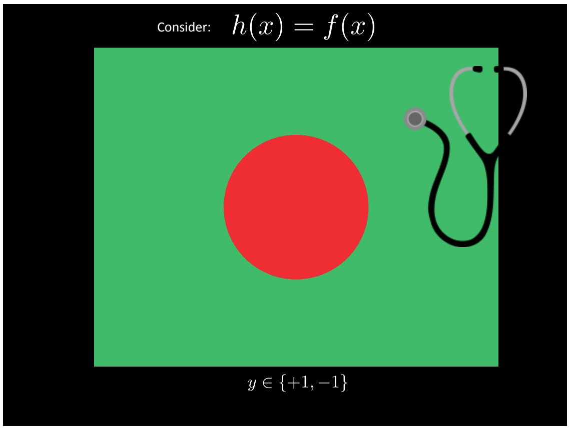

$y = f(x)$
$y \in \{+1, -1\}$

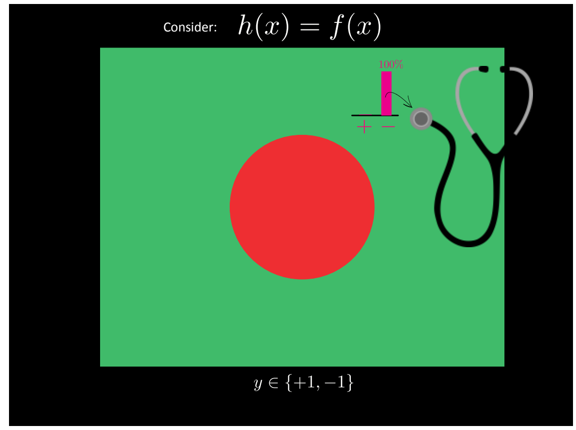

S_1

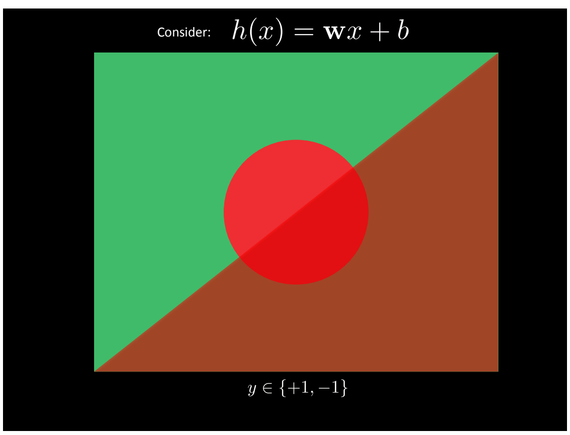

S_2

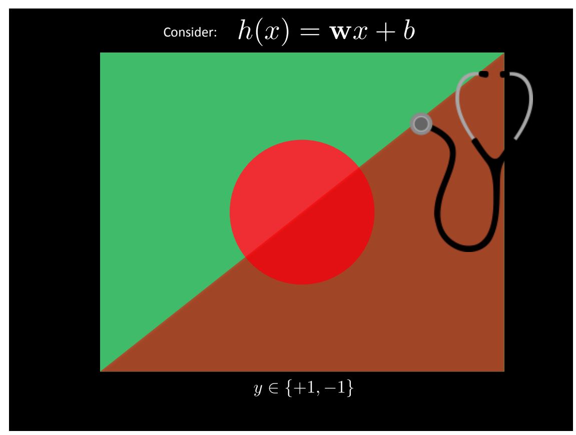

S_3

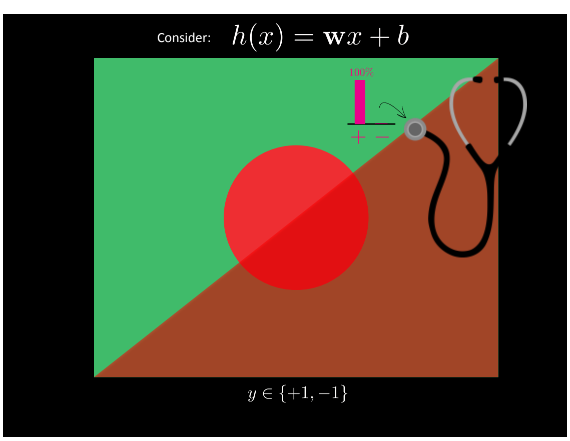

S_4











$$\mathbb{E}_S\left[(y_i - h_S(x_i))^2\right] =$$

$$(y_i - \mathbb{E}_S[h_S(x_i)])^2 \; +$$

$$+ \; \mathbb{E}_S[(h_s(x_i) - \mathbb{E}_S[(h_S(x_i))])^2]$$

Label Noise

Noise-free:

$$y_i = f(x_i)$$

Regression:

$$y_i = f(x_i) + noise$$
$$y_i = f(x_i) + \mathcal{N}(0, \sigma^2)$$

Classification:

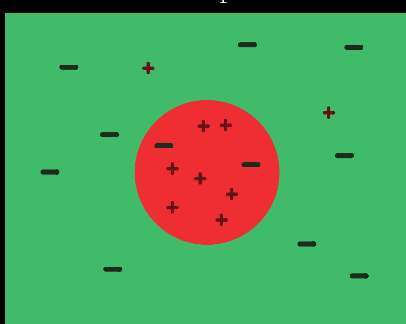
$$y_i = noisy(f(x_i))$$

(*noisy()* switches label with probability *p*)

$y = \text{noisy}(f(x))$ (flip sign with probability 0.25)

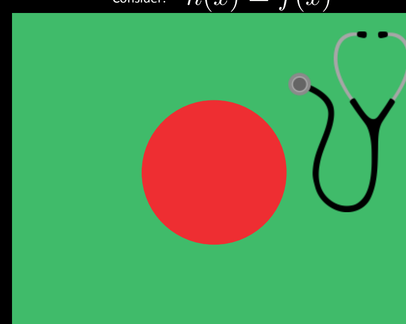
$y \in \{+1, -1\}$

S_1



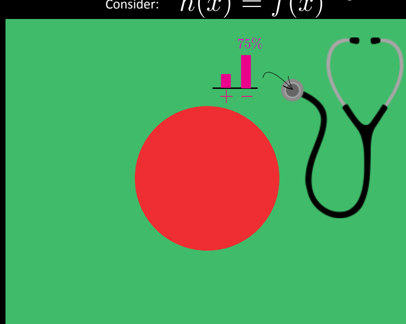
$y \in \{+1, -1\}$

Consider: $h(x) = f(x)$ $y = \text{noisy}(f(x))$



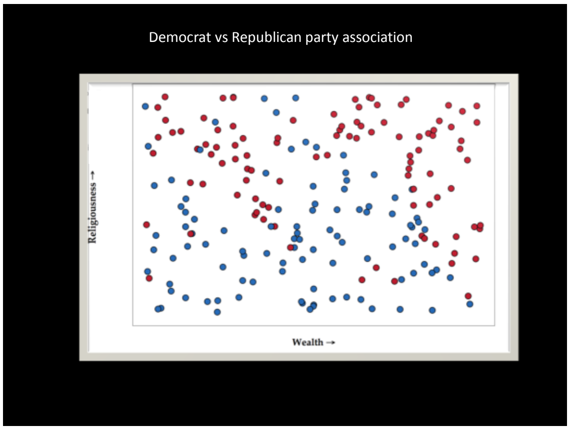
$y \in \{+1, -1\}$

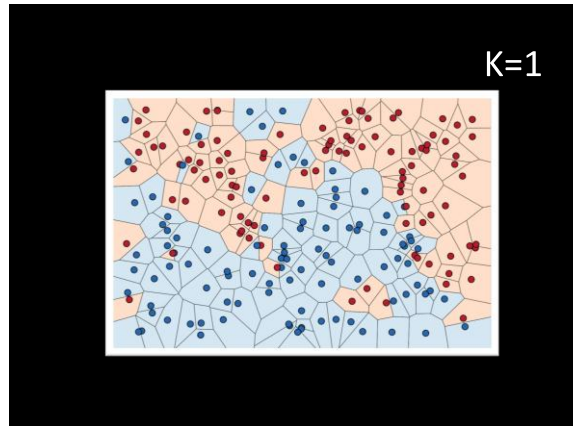
Consider: $h(x) = f(x)$ $y = \text{noisy}(f(x))$

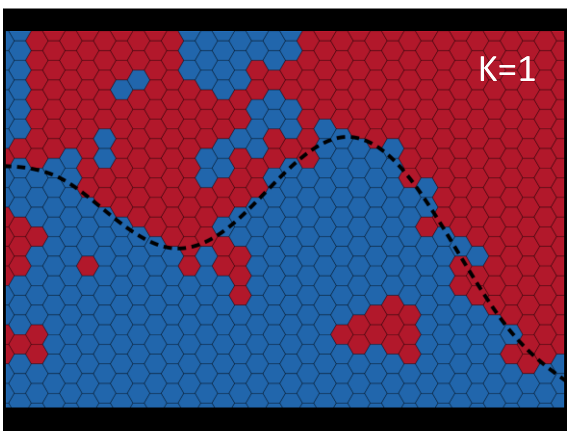


$y \in \{+1, -1\}$

Example
(kNN)


Democrat vs Republican party association
Religiousness →
Wealth →


K=1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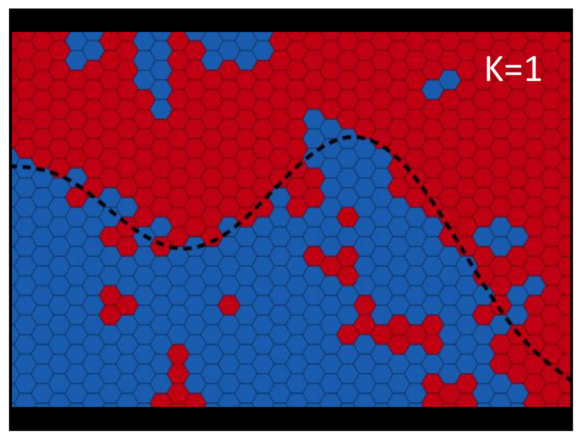
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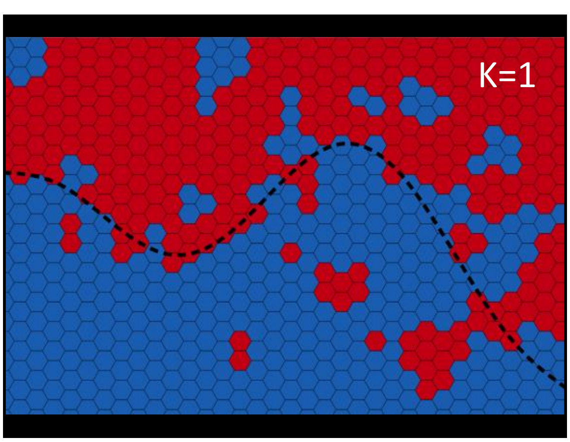
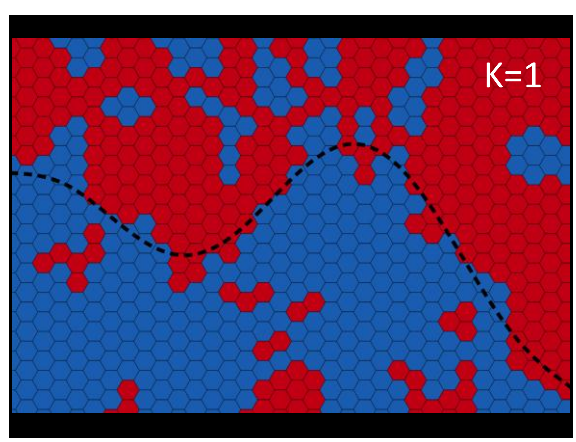

K=1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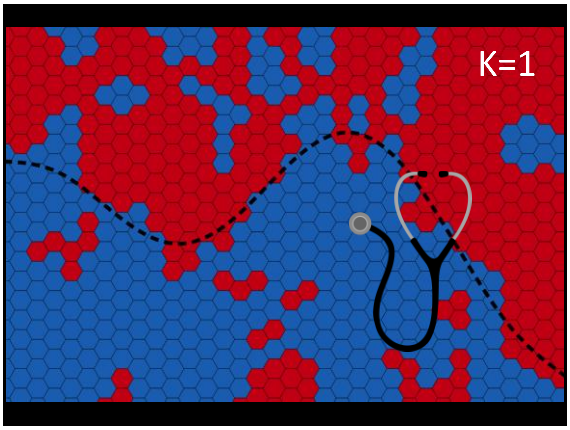
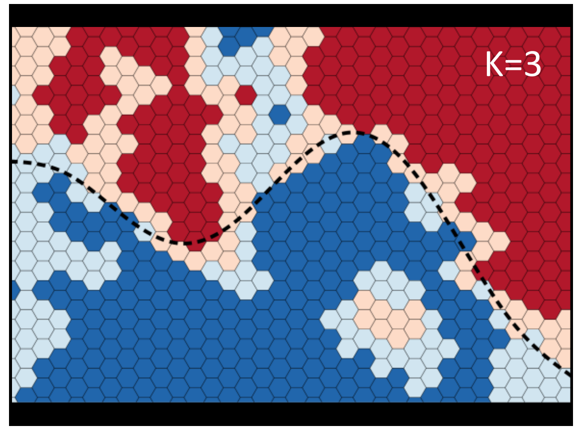
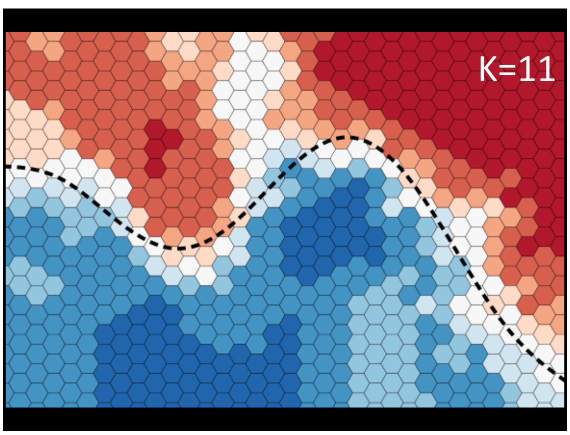
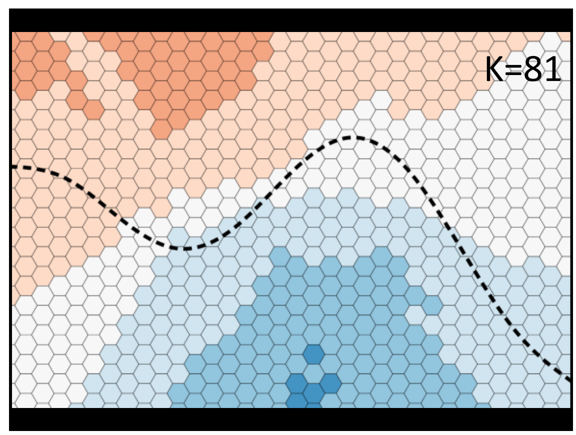
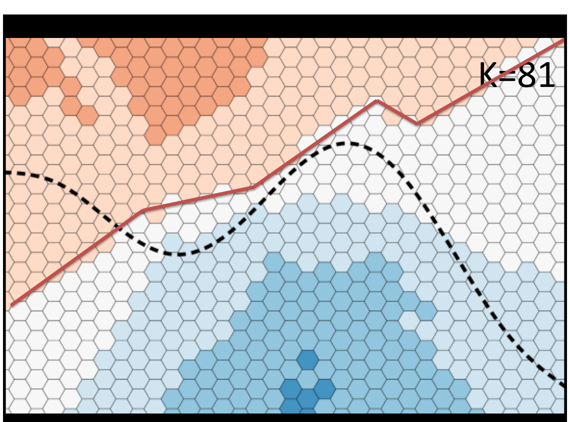

K=1


K=3


K=11


K=81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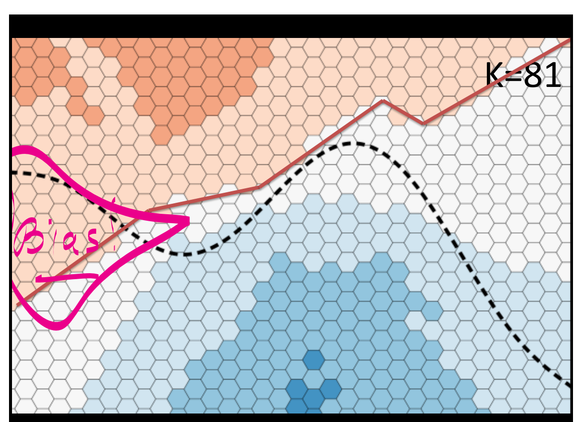
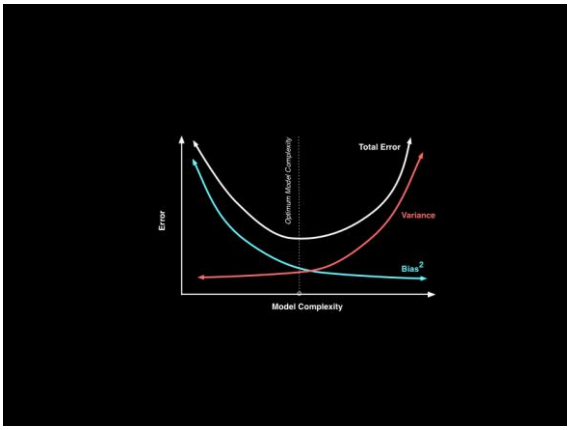
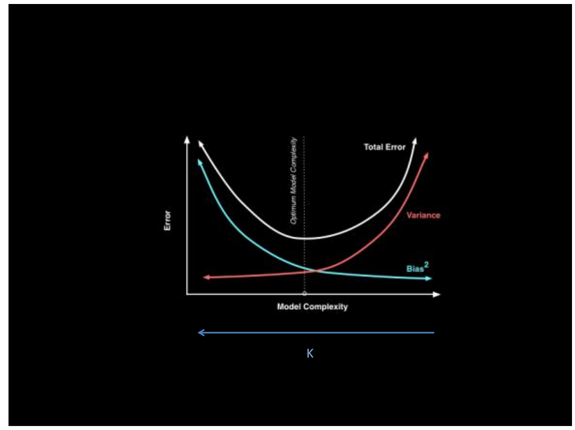
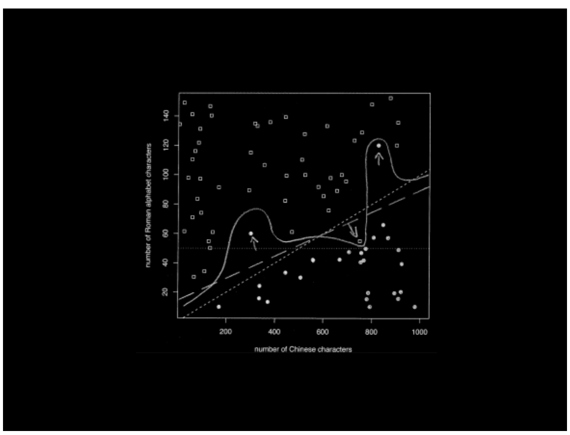

K=81
Bias!







CLAIM:

$$\mathbb{E}_S\left[(y_i - h_S(x_i))^2\right] =$$

bias² $(y_i - \mathbb{E}_S[h_S(x_i)])^2 \; +$

variance $+\, \mathbb{E}_S[(h_s(x_i) - \mathbb{E}_S[(h_S(x_i))])^2]$

USEFUL LEMMA:

$$\mathbb{E}[(\alpha - \mathbb{E}[\alpha])^2] = \mathbb{E}[\alpha^2] + \mathbb{E}[\alpha]^2$$

$$y_i = f(x_i) + \mathcal{N}(0, \sigma^2)$$

$$\mathbb{E}_S\left[(y_i - h_S(x_i))^2\right] =$$

bias² $(y_i - \mathbb{E}_S[h_S(x_i)])^2 \; +$

variance $+\, \mathbb{E}_S[(h_s(x_i) - \mathbb{E}_S[(h_S(x_i))])^2]$

$$y_i = f(x_i) + \mathcal{N}(0, \sigma^2)$$

$$\mathbb{E}_S\left[(y_i - h_S(x_i))^2\right] =$$

bias² $\quad (f(x_i) - \mathbb{E}_S[h_S(x_i)])^2 +$

variance $\quad + \mathbb{E}_S[(h_s(x_i) - \mathbb{E}_S[(h_S(x_i))])^2]$

noise $\quad + \mathbb{E}_S[(f(x_i) - y_i)^2]$

$$y_i = f(x_i) + \mathcal{N}(0, \sigma^2)$$

$$\mathbb{E}_S\left[(y_i - h_S(x_i))^2\right] =$$

bias² $\quad (f(x_i) - \mathbb{E}_S[h_S(x_i)])^2 +$

variance $\quad + \mathbb{E}_S[(h_s(x_i) - \mathbb{E}_S[(h_S(x_i))])^2]$

noise $\quad + \sigma^2$

$$\mathbb{E}_S\left[(y_i - h_S(x_i))^2\right] =$$

bias² $\quad (y_i - \mathbb{E}_S[h_S(x_i)])^2 +$

variance $\quad + \mathbb{E}_S[(h_s(x_i) - \mathbb{E}_S[(h_S(x_i))])^2]$

BAGGING

revisited

Bagging

(Breiman, 1996)

Bagging (Boostrap aggregating).

```
BAGGING(S = ((x_1, y_1), ..., (x_m, y_m)))
  for t ← 1 to T do
      S_t ← BOOTSTRAP(S) ▷ i.i.d. sampling with replacement from S.
      h_t ← TRAINCLASSIFIER(S_t)
  return h_S = x ↦ MAJORITYVOTE((h_1(x), ..., h_T(x)))
```

Why does it work?

Bagging

Ensemble :

$$h_S(x) = \text{sign}\left(\sum_{t=1}^{T} \alpha_t h_t(x)\right)$$

Bagging : Special case where we fix:

$$\alpha_t = 1 \quad \text{and} \quad h_t = \mathbb{L}(S_t)^*$$

* $\mathbb{L}$ is some learning algorithm

S_t is a training set drawn from distribution $P(<x,y>)$

Bagging

Bagging Ensemble :

$$h_S(x) = \text{sign}\left(\sum_{t=1}^{T} h_t(x)\right)$$

What happens to *bias* and *variance?*

Bagging

Bagging Ensemble (regression) :

$$h_S(x) = \frac{1}{T}\sum_{t=1}^{T} h_t(x)$$

bias² $(y_i - \mathbb{E}_S[h_S(x_i)])^2$

variance $\mathbb{E}_S[(h_s(x_i) - \mathbb{E}_S[(h_S(x_i))])^2]$

Bagging

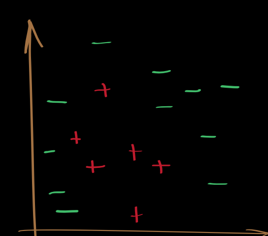
What happens to *bias* and *variance?*

$$\text{Bias}(h_s, x_i) =$$

$$\text{Var}(h_s, x_i) \approx$$

Bagging has approximately the same bias, but reduces variance of individual classifiers!

Bagging



Bagging as a "Training set manipulator"

Bagging as a "Training set manipulator"

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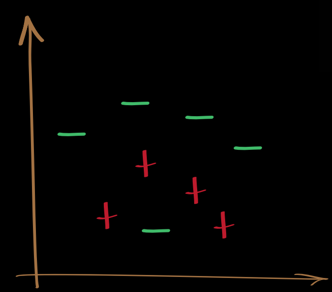
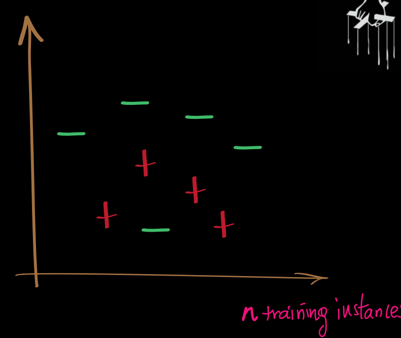
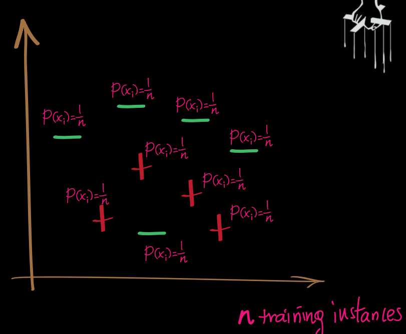


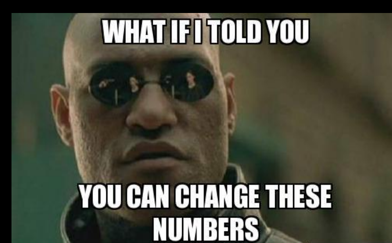
Bagging as a "Training set manipulator"



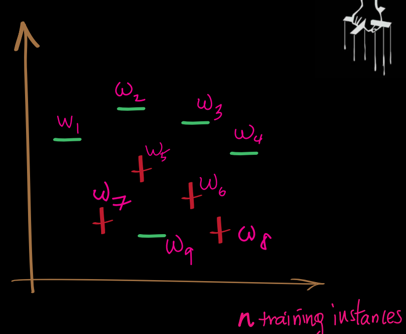
Bagging as a "Training set manipulator"



Bagging as a "Training set manipulator"



Bagging as a "Training set manipulator"



Ensemble

Problem : given T binary classification hypotheses (h_1,..., h_T), **find** a combined classifier:

$$h_S(x) = \text{sign}\left(\sum_{t=1}^{T} \alpha_t h_t(x)\right)$$

with better performance.

Teaser